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PART II

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POLLUTANT PRODUCTION IN A SIMULATED TURBOJET AFTERBURNER

Part II. COMPUTER PROGRAM FOR CALCULATION OF POLLUTANT HISTORY IN AFTERBURNING TURBOJET ENGINES

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The University of Tennessee Space Institute

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Air Force Aero Propulsion Laboratory
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71

POLLUTANT PRODUCTION IN A SIMULATED TURBOJET AFTERBURNER
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FOREWORD

This research program was initiated 1 November 1970 under USAF Contract F33615-71-C-1125. The work was performed between 1 November 1970 and 31 July 1971 by The University of Tennessee Space Institute, Tullahoma, Tennessee, and administered by the Air Force Aero Propulsion Laboratory, Wright-Patterson Air Force Base, Ohio, Mr. Kenneth N. Hopkins (AFAPL/TBC), Project Engineer. The contract was initiated under Project 3066, "Gas Turbine Technology," Task 306605 "Combustion Systems Performance and Stability."

Scientific and engineering personnel of the Space Institute, identified as "et al." on the cover, who engaged in the experimental work and preparation of this report, are:

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The authors wish to express sincere appreciation to Mr. R. Kamm, Special Assistant to Dr. Goethert, for his active cooperation in the project; to Mr. R. Nygaard, Engineer, and to Mr. J. Goodman, Mr. J. Boazman, and Mr. J. Rothert, Technicians, for their cooperation and assistance in the Combustion Laboratory; to the personnel at ESF and CCO of ARO, Inc., especially Mr. J. McCabe and Mr. W. Armstrong, for their cooperation.

This report was submitted by the authors in August, 1971.

This report is bound in two parts. Part I contains technical details of the report. Part II consists of a User's Manual for the computer program developed for calculating pollutant production in a turbojet afterburner.

The program has been operated on the IBM 370/155 using FORTRAN IV G Level 18. To keep within B partition it was necessary to overlay INIT with INTEG, SETUP, SETYP, SETHP, GAUSS. All pages of this manual are effective 31 July 1971.

Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

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ABSTRACT

An experimental and theoretical study has been made of the history of the pollutants carbon monoxide (CO), unburned hydrocarbons (HC) and nitrogen oxides (NO_x) in a turbojet afterburner. Experimental traverses at several axial stations were performed in a simulated afterburner in which exhaust from a J-47 combustor can, operated at medium power, was mixed with fuel spray. Experiments were carried out both in a non-bypass and in a bypass configuration (secondary air was mixed with primary exhaust). The non-bypass tests were carried out at high combustor efficiency, and yielded the following: CO = 300 ppm, HC less than 10 ppm, NO_x = 100 ppm. In the bypass tests, fuel distribution was nonuniform and combustor efficiency was low. The concentrations obtained were CO = 10,000 ppm, HC = 1000 ppm, NO_x = 100 ppm. The theoretical analysis consisted of a computer program for reacting flow with turbulent mixing. The computer program was very slow and therefore of limited usefulness in terms of cost and questionable results, since it could not be checked against experiment Infrared measurements of NO in the combustion tunnel were attempted. Indications were obtained of NO at the 5.3 micron band, but quantitative measurements were not obtained.

TABLE OF CONTENTS

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GLOSSARY

R	Radial position - inches
T	Temperature - °K
S	Temperature - °R
U	Velocity - ft/sec
Y	Species mass fractions
ROU	Mass flux - lb/(sec sq. ft.)
PSI	Stream function $\sqrt{(lb/sec)}$
UPR	Velocity at previous location - ft/sec
YPR	Species mass fraction at previous location
HST	Static enthalpy Btu/lb
HT	Total enthalpy Btu/lb
TPR	Temperature at previous location °R
HTPR	Total enthalpy at previous location Btu/lb
CM	Molecular weight (average)
X	Mole fraction
H	Species chemical enthalpy Btu/lb mole
W	Species production rate lb/lb
E	Species production per lb/lb ft
YO	Initial fuel mass fraction
TO	Time since start of burning
TAU	Burning time
ISP	Number of species
IRE	Number of reactions
IMU	IMU-5 = Number of 3 body reactions
UM	Turbulent viscosity lb/ft sec

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SECTION I

INTRODUCTION

This users manual was prepared under contract number F33615-71-C-1125, and represents Item Number 0001 Sequence Number A002 under requirements of that contract. The purpose of writing the computer program was to provide the Air Force with a means of estimating air pollution concentrations in the exhaust gases from afterburning turbojet engines.

SECTION II

COMPUTER PROGRAM SYSTEM CAPABILITIES

2.1 PURPOSE

The purpose of this computer program is to solve the partial differential equations of change for momentum, species, and enthalpy, to obtain radial and axial profiles of velocity, temperature, and species concentrations in a turbulent reacting fluid. A finite difference approximation to the equations is made.

The chemical species considered and chemical reactions involved are those pertinent to burning of a liquid hydrocarbon fuel in a hot exhaust gas from a primary combustor. By controlling the input a calculation of the mixing and combustion in a bypass type engine may also be made. While the primary purpose of the research has been to estimate levels of the pollutants NO, CO, and unburned hydrocarbons, in exhaust gases, the levels of several other species must be taken into account in order to calculate pollutant levels.

2.2 GENERAL DESCRIPTION OF THE SYSTEM

A FORTRAN program has been written to achieve the purpose described above. The differential equations, transformed from (length, radius), to (length, stream function) coordinates, have been approximated by finite difference equations.

Initially, certain thermodynamic data for the chemical species are read, followed by data necessary to calculate chemical reaction rates. Then, initial data of temperature, velocity, and species concentrations as a function of radial position in an axisymmetric flow are read in. The program does not read any more data.

From the initial profiles as a function of radius, a conversion to the stream function variable is made, with appropriate interpolation.

An iteration scheme is used to solve for dependent variables (velocity, enthalpy, species concentration) as a function of axial distance. The program proceeds stepwise from the initial condition, until a maximum axial distance is reached. The outer boundary condition is an inviscid reacting flow. When the flow variables at the stream function location adjacent to the inviscid flow deviate from the inviscid flow by 1 part in 10^4, the viscous flow region is expanded by one step in stream function. The number of stream function

steps is allowed to increase to 50, if necessary. If more expansion is needed, the stream function step size is doubled, and number of steps is halved. This process repeats itself as necessary.

2.3 FUNCTIONS PERFORMED

There are 13 subdivisions of the program.

1. MAIN Program
2. Subroutine SPECIE (KK1, KK2, NU)
3. Subroutine THERMO (KRIS, JA, IT)
4. Subroutine INIT
5. Subroutine TRANSP (NLOW, NHIGH)
6. Subroutine INTEG (NLOW, NHIGH, IN)
7. Subroutine SETUP (RUP)
8. Subroutine SETYP (RUP)
9. Subroutine SETHP (RUP)
10. Subroutine GAUSS
11. Subroutine CHANGE (RUP)
12. Subroutine PRINT (KUSK,KUN)
13. Subroutine CHEMIE (KRYS, KRAS, IJ)

The MAIN program controls the flow of information, causing THERMO, CHEMIE, and INIT to read in initial data. It then proceeds with the computation and prints out results at every 50th axial station, until stopped by either reaching the maximum desired axial distance (ZMAX feet) or exceeding the time limitation.

2.4 FUNCTION DESCRIPTIONS

2.4.1 Main Program

Summary of Operations performed by MAIN

The main program first sets certain parameters, namely ISP = 14, IRE = 17, IMU = 11, which are in labelled common ZZZ. There are, respectively, the number of species, the number of reactions, and the number of the last reaction which involves three bodies (see CHEMIE). In addition, the variable TAU is set equal to $.4 \times 10^{-3}$, which is the hydrocarbon burning time in seconds. TAU is in labeled common XXX. Certain other parameters are also set, so as to cause THERMO to read thermodynamic data, and CHEMIE to read chemical reaction rate data. The main program then calls upon INIT to read in velocity, temperature, and species concentrations as a function of radius. The first item actually read is NNN, which defines the number of radial locations considered. INIT converts the indepen-

dent variable from radius to stream function, and interpolates to obtain initial dependent variables, velocity, temperature, and species concentrations, at equal intervals of stream function. The stream function interval is denoted by DPSI. DELX is the interval in feet, and is defined to be .00001. RUP = DELX/DPSI**2 is defined. XMAX = 0.7 (feet) is defined as the maximum axial distance to be considered.

The main program calls upon SPECIE to calculate mole fractions, molecular weights, and mass fluxes at all radial locations, and calls upon THERMO to calculate static enthalpies of the species. Total enthalpies are calculated. The TRANSP subprogram is called upon to calculate a turbulent viscosity, and INTEG to calculate radius as a function of stream function, and also to calculate certain coefficients (AP, APR) needed for subsequent finite difference calculations.

The main program writes the data on initial profiles as a function of stream function. It then proceeds in a stepwise fashion to calculate the flow variables as a function of axial location.

After the writing of the initial data, there is very little necessity or possibility for operator or programmer intervention in the main program. The number of radial locations, NNN, is a major variable which is controlled initially and internally. The variables IK and IA define the locations of the inner and outer bounds of the viscous flow region. In the present application, the inner bound is taken to be the center-line. The outer bound is always IA = NNN-1. Species calculations run from 1 to ISP, which is defined previously.

A variable KUSK defines the number ofiterationswhich have been performed at an axial location. The iterations stop after KUSK = 3. Prior to the start of calculations, the axial position, Z, is incremented. IA is checked to see if the maximum number of streamlines permitted has been reached. If IA = NILS - 1, a doubling of stream function step size is incurred, together with a reduction of the number of steps considered. This is done through the subroutine CHANGE. In the present program, NILS = 51 is defined as data. NILS must be odd. The resulting profiles are written after CHANGE.

Whether or not a change occurs, the boundary values at NNN are calculated at the incremented axial position. The boundary value for velocity, UEO = U(NNN) never changes since the inviscid flow is considered to occur at constant pressure. The velocities at the other radial locations are calculated through SETUP and GAUSS. If |(U(IA) - UEO)/UEO| > TOL, an indicator, IAP is set up to tell the program to increase the viscous region (this is not done until after all iterations are complete). The species concentrations are calculated at NNN, and then in the viscous region through SETUP and GAUSS. If the relative difference in molecular weights at IA and NNN exceeds TOL, the indicator IAP is set. The total enthalpy at NNN, HT(NNN) = HEO is constant in the inviscid flow. In the viscous region, new

total enthalpies, HT(I) are calculated through SETUP and GAUSS. If the relative difference in total enthalpies at IA and NNN exceeds TOL, the indicater IAP is set.

In the first interation, species production terms at the previous location are used. In the second and third iterations the species production terms at the midpoint of the interval are approximated by a Taylors series expansion. The same process of calculating boundary values, then viscous flow values, of the flow variables is followed. In between iterations, TRANSP and INTEG are called upon to obtain improved values of turbulent viscosity and the terms AP, APR used in SETUP, SETYP, SETHP.

After the third iteration, IAP is checked to see if the flow field should be expanded. If it should be it is expanded. If it should not, previous values of the flow variables are identified, and the program returns to increment another axial step. The results are printed every 50 steps, as defined by the variable KYS. KYS is set to 50 near the start of the main program. If this causes too much printing, KYS could be set to a larger value.

Inputs to MAIN

There are no inputs read into MAIN by tape, cards, etc.

Expected Outputs

After INIT, the MAIN program writes initial profiles of selected flow variables as a function of stream function.

After CHANGE, the MAIN program writes resultant profiles of selected flow variables.

Other writing is done by other subroutines.

2.4.2 SPECIE (KK1, KK2, NU)

Purpose and Uses of SPECIE

SPECIE is capable of calculating CM(I) (average molecular weight), X(J,I) (mole fractions of ISP species) and ROU(I) (mass flux), from axial location KK1 to KK2

If NU = 0, CM(I) and X(J,I) are transmitted
If NU < 0, ROU(I) is also transmitted
If NU = 0, only ROU(I) is transmitted

Inputs

There are no system inputs on cards or tape to SPECIE

Expected output

There are no system outputs on cards or tape from SPECIE

2.4.3 THERMO (KRIS, JA, IT)

Summary of Operations Performed by THERMO

In the initial phases of the program, JA is set to be greater than zero, which causes THERMO to read in coefficients for calculating species enthalpies. When JA is less than or equal to zero, and KRIS equals 100, species enthalpies are calculated at T(IT) (temperature allocation IT); if KRIS is different from 100, temperature is determined at a static enthalpy HST(IT), by means of a Newton-Raphson process.

System Inputs

A total of ISP sets of coefficients A, followed by ISP coefficients B. These are, respectively, the 300-1000°K and 1000-5000°K coefficients a_1 - a_0 from Table V of NASA SP-3001, for the appropriate compounds. For fuel, a value of -23900R calories per gram mole of $C_{10}H_{22}$ has been estimated to be the enthalpy of fuel at 477°F (estimated boiling point) from the elements at 298°K. The program also reads SENS, heats of formation at 298°K. These are not used in the present program.

System Outputs

The coefficients B are printed after being read in.

2.4.4 INIT

Summary of Operations Performed by INIT

INIT is called only once. It reads in NNN, the number of streamlines considered, then NNN cards containing UE(I) (velocity) SE(I) (temperature) and R(I) (radius) with R(I) starting at zero and increasing monotonically. Initial profiles of species mass fractions (YE(J,I)) are then read in at R(I). Stream functions are calculated for the initial profile, and the data are interpolated to equal intervals of stream function with the interval DPSI = PSI/(NNN-1), where PSI(I) is the value of stream function at location I.

System Inputs

NNN is an integer less than or equal to NILS (main program). UE(I) is in feet per second, SE(E) in degrees , Rankine, R(I) in inches. Species mass fractions are introduced per card up to ISP, for each R(I)

System Outputs

Nothing is written on card or tape from INIT.

2.4.5 TRANSP (NLOW, NHIGH)

Summary of Operations Performed by TRANSP

TRANSP calculates a turbulent viscosity, UM, according to Schetz's displacement thickness model, as described in the report. A DATA statement defines RJ, an inner jet radius, in feet.

System Inputs and Outputs

Nothing is read or written by TRANSP.

2.4.6 INTEG (NLOW, NHIGH, IN)

Summary of Operations Performed by INTEG

INTEG calculates radial values (R1I) as a function of stream function. It also calculates AP(I) and APR(I) at locations NLOW to NHIGH.

If IN = 0, AP = APR = SP

If IN is not zero, AP = .5 (SP + APR)

where SP = UM * R(I) **2 * ROU(I)/PSI(I)

is a term which arises in the transformation of equations to stream function coordinates.

System Inputs and Outputs.

No information is read to or written from INTEG.

2.4.7 SETUP (RUP)

Summary of Operations Performed by SETUP

SETUP calculates coefficients for solution of the finite difference equations for velocity. These are transmitted to labelled COMMON UPSET and used by GAUSS. The indicator KOR is set equal to -10.

System Inputs and Outputs

There are no INPUT/OUTPUT Statements in SETUP.

2.4.8 SETYP (RUP)

Summary of Operations Performed by SETYP

SETYP calculates coefficients for solution of the finite difference equations for species mass fractions, to be used by GAUSS. The indicator KOR is set to 0. A DATA statement defines CN which is the inverse of the turbulent Prandtl number. CN is taken to be 1 in the present study.

System Inputs and Outputs

There are no INPUT/OUTPUT Statements in SETYP.

2.4.9 SETHP (RUP)

Summary of Operations Performed by SETHP

SETHP calculates coefficients for solution of the finite difference equations for total enthalpy, to be used by GAUSS. The indicator KCR is set to + 10. A DATA statement sets CN = 1 as in SETYP, in the present program.

System Inputs and Outputs

There are no INPUT/OUTPUT statements in SETHP.

2.4.10 GAUSS

Summary of Operations Performed by GAUSS

Depending on whether KOR (see previous three subroutines) is negative, zero, or positive, GAUSS solves for velocity (U), species mass fractions (Y(J,I)) or total enthalpy (HT) through the viscous flow field. When KOR = 0, the mole fractions (X(J,I)) and average molecular weights (CM) are also determined. When KOR is positive, static enthalpy (HST) is also determined. In addition, GAUSS determines the outermost location at which the flow variables U, CM, HT deviate significantly from the inviscid external flow. This is defined to be IAP, as discussed in MAIN.

The highest location at which significant deviation occurs in each branch is defined to be NO(I), I = 1, 2, 3. Quantities NE(I), defining the innermost location at which the flow variables deviate significantly from an inviscid center flow, are also defined but are not used in the present program. An inner, reacting, inviscid flow could not be included in the program without some modification (essentially everything done in the stepwise calculations at NNN would have to be done at the inner boundary). An inner equilibrium flow could be included with slight modification.

The "significant deviation" mentioned above is defined in DATA as TOL, and is taken to be $1. \times 10^{-4}$ in the present program.

System Inputs and Outputs

There are no INPUT/OUTPUT statements in GAUSS.

2.4.11 CHANGE (RUP)

Summary of Operations Performed by CHANGE

CHANGE is called upon when the viscous flow field has expanded to its maximum size. The value of DPSI (stream function step size) is doubled, and the number of intervals is halved. In the present program, NNN is reduced from 51 to 26. Values of the flow variables are also transferred so that the flow variables correspond to the proper stream function values.

System Inputs and Outputs

There are no INPUT Statements in CHANGE. A printed output indicates that the number of points has been halved, and gives values of certain variables which are the distance downstream from the start in inches, and the distance interval in inches. The values are duplicated because at one time, DELX was changed when DPSI was changed. This is no longer done.

2.4.12 PRINT (KUSK, KUN)

Summary of Operations Performed by PRINT

PRINT lists pertinent variables when called upon by the MAIN program.

System Output

The first data listed are

Z(feet), ZX(inches), DELX(feet), DPSI, NEL, NEU, IA, KUSK, KUN

Then at each of NNN locations, I(radial location), PSI, R, S(Temperature in °R) AP, APR, HT in one line, followed by Y(I,J) (2 lines) W(I,J) (2 lines) E(I,J) (2 lines) and a final line with YTOT, CM, ROU. This output represents the fundamental output for the program.

2.4.13 CHEMIE (KRYS, KRAS, IT)

Purpose and Uses of CHEMIE

This subroutine calculates quantities necessary to calculate the species production terms for inclusion in the species conservation equations. It also reads in the parameters for calculating reaction rates. If (KRYS + KRAS) is not less than zero, the parameters for the reactions rates are read in and listed. If (KRYS + KRAS) is less than zero, the reaction rates, species production, and linearization terms are calculated. If KRAS is greater than zero, species production terms (W) are calculated.

If KRAS is equal to zero, linearized terms are calculated.

The reactions considered are:

$$H + O_2 = O + OH \quad (1)$$

$$H_2 + O = OH + H \quad (2)$$

$$H_2 + OH = H + H_2O \quad (3)$$

$$OH + OH = H_2O + O \quad (4)$$

$$H_2 + M = H + H + M \quad (5)$$

$$H_2O + M = H + OH + M \quad (6)$$

$$N_2 + M = N + N + M \quad (7)$$

$$O_2 + M = O + O + M \quad (8)$$

$$NO + M = N + O + M \quad (9)$$

$$N_2O + M = N_2 + O + M \quad (10)$$

$$NO_2 + M = NO + O + M \quad (11)$$

$$CO + OH = CO_2 + H \quad (12)$$

$$NO + O = N + O_2 \quad (13)$$

$$NO + N = N_2 + O \quad (14)$$

$$NO + O_2 = NO_2 + O \quad (15)$$

$$NO + NO = N_2O + O \quad (16)$$

$$C_nH_{2n+2} + \frac{n}{2} O_2 \rightarrow nCO + (n+1) H_2 \quad (17)$$

System Inputs and Outputs

When called upon near the start of the program, CHEMIE reads data for calculating chemical reaction rates. These are, in order,

CW	(molecular weights)
AU	(collision terms in forward rate constants)
CU	(collision terms in backward reaction rate constants)
E	(forward rate activation energy/R)
D	(backward rate activation energy/R)
GNUF(I,J)	(stoichiometric coefficients for species I in forward reaction J)
GNUB(I,J)	(stoichiometric coefficients for species I in backward reaction J)
AF, BF, AB, BB	(respectively; temperature coefficient density coefficient for forward reaction, similarly for reverse)
EN	(number of carbon atoms in fuel $C_n H_{2n+2}$)

Certain of the above are listed after being read in, namely, CW, AU, CU, E, D, GNUF, GNUB.

2.5 Usage Instructions

2.5.1 Preparation of Inputs

Titles and Description of Inputs

The basic inputs to the program, initial profiles, are read by the subroutine INIT. The titles of the inputs, read in INIT, are

NNN - Number of inputs, number of streamlines considered initially.

UE, SE, R - One set per card.

UE is specified initial velocity, (ft/sec); specified initial temperature (degrees Rankin); at R, radial position in inches.

YE(J,I) A total of ISP species mass fractions, arranged in the order, H, O, H_2O, OH, O_2, H_2, N_2, N, NO, N_2O, NO_2, CO, CO_2, fuel at R. This requires two cards for the present value of ISP = 14.

The data are read on cards.

The cards must be read in the sequency:

NNN Card

UE, SE, R - Total of NNN cards

YE - One set of cards for each R (2 NNN cards in the present program).

Limitations

The first R is taken to be zero. R must increase from card to card. Negative values for any variable would have no physical meaning.

Formats

```
READ(5,100) NNN
READ(5,101)(UE(L),SE(L),R(L),L=1,NNN)
READ(5,102)((YE(J,I),J=1,ISP),I=1,NNN)

100 FORMAT(I5)
101 FORMAT(3F10.0)
102 FORMAT(7D10.0)
```

Relationship of Inputs to Outputs

These are the fundamental starting values for the differentail equations. All output profiles are related to these.

In particular, selected flow variables are printed in MAIN directly after INIT. These are dependent on PSI, rather than R, as are all subsequent outputs of flow variables. Only values at the end points should be the same.

2.5.2 Results of Operation

Description of Results

The major results are profiles of velocity, temperature, and species mass fraction at specified axial locations. The output comes on the printer.

Format and Content

The output instruction and format are as follows

```
      Z=ZX/12.
      WRITE (6,30) Z,ZX,DELX,DPSI,NEL,NEU,IKS,KUSK,KUN
      DO 20 I=IK,IA
      YTOT=0.0
      DO 10 J=1,ISP
10    YTOT=YTOT+Y(J,I)
      WRITE (6,40) I,PSI(I),R(I),S(I),U(I),AP(I),APR(I),HT(I)
      WRITE (6,50) I,(Y(J,I),J=1,ISP)
      WRITE (6,50) I,(W(J,I),J=1,ISP)
      WRITE (6,50) I,(E(J,I),J=1,ISP)
      WRITE (6,60) I,YTOT,CM(I),ROU(I)
20    CONTINUE
      WRITE(6,60) KQ,UM
      RETURN
C
30    FORMAT ('1',////,4(2X,F15.10),5(3X,I5),7H OUTPUT,///)
40    FORMAT (/,2X,I4,7(2X,E14.7))
50    FORMAT (2X,I4,7(2X,E14.7)/,6X,7(2X,E14.7))
60    FORMAT (2X,I4,3(2X,E14.7))
```

Use of Outputs

The outputs contain information on the pollutant concentrations, and other concentrations. Hence the use of output, at the end of the afterburner, will be to predict pollutant concentrations. Intermediate results indicate the evolution of the pollutants.

A Sample input is presented in this and the following page

27		
286.	2145.	0.
286.	2145.	.184
286.	2145.	.368
285.	2140.	.552
282.	2136.	.736
278.	2130.	.92
270.	2120.	1.104
262.	2110.	1.288
258.	2100.	1.472
254.	2088.	1.656
250.	2076.	1.84
246.	2062.	2.024
242.	2050.	2.208
238.	2038.	2.392
234.	2022.	2.576
232.	2004.	2.76
230.	1980.	2.944
228.	1950.	3.128
226.	1910.	3.312
224.	1872.	3.496
223.	1840.	3.68
223.	1830.	3.864
223.	1830.	4.048
223.	1830.	4.232
223.	1830.	4.416
223.	1830.	4.6
223.	1830.	4.784

```
.000000700.000001000.029600000.000001000.167800000.000001600.707400000
.000000001.000030601.000000700.000000700.000285000.065800000.029000000
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.000000001.000030601.000000700.000000700.000285000.065800000.027000000
.000000700.000001000.029600000.000001000.167800000.000001600.709600000
.000000001.000030601.000000700.000000700.000285000.065800000.026800000
.000000700.000001000.029600000.000001000.167800000.000001600.709800000
.000000001.000030601.000000700.000000700.000285000.065800000.026600000
.000000700.000001000.029600000.000001000.167800000.000001600.710000000
.000000001.000030601.000000700.000000700.000285000.065800000.026400000
.000000700.000001000.029600000.000001000.167800000.000001600.710200000
.000000001.000030601.000000700.000000700.000285000.065800000.026200000
.000000700.000001000.029600000.000001000.167800000.000001600.710400000
.000000001.000030601.000000700.000000700.000285000.065800000.026000000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
.000000700.000001000.029600000.000001000.167800000.000001600.710600000
.000000001.000030601.000000700.000000700.000285000.065800000.025800000
```

2.6 Operating Instructions

2.6.1 Operating Procedures

Initiation of Program

The program is on cards, together with data. For a particular computer, proper control cards must be introduced. Input is on cards, output on printer.

Maintaining Computer Program Operation

The program will continue to operate, as long as too large a step size is not used. If too large a step size is used, the procedure is unstable, and is characterized by logs of negative numbers, due to temperature going negative. The program must be started with a smaller step size (DELX).

Termination and Restart

Termination is achieved when Z > ZMAX. If interruption of the program is necessary, some subroutine would have to be written to identify the necessity for interruption at statement 40, MAIN, store program and all data, and restart at the same point.

2.6.2 Operator Inputs

Initial imputs, other than the basic initial profile mentioned previously, include the thermodynamic and chemical data initially read in THERMO and CHEMIE.

The input statements and formats, and data used in the present version, are shown below.

In THERMO

```
  180   READ (5,260) ((A(K,J),K=1,6),J=1,ISP)
        DO 190 J=1,ISP
        READ (5,260) (B(K,J),K=1,6)
        WRITE (6,280) (B(K,J),K=1,6)
  190   CONTINUE
        READ (5,270) (SENS(J),J=1,ISP)
        GO TO 170
  200   WRITE (6,210) M,R(M),PSI(M),HST(M),HTS,FA,FB,TP,T(M)
        GO TO 90
C
  210   FORMAT (///,2X,I4,8(2X,E13.5),1X,4HTHER,///)
  220   FORMAT (/,2(2X,I5),6(2X,E15.8))
  230   FORMAT (2X,I5,4(2X,E15.8))
  240   FORMAT (2X,I5,7(2X,E15.8))
  250   FORMAT (2X,I5,7(2X,E15.8),/)
  260   FORMAT (4D15.8,/2D15.8)
  270   FORMAT (7D10.0)
  280   FORMAT (/////,1X,6E20.8,/////)
```

The Data used in the present version are as follows:

```
 0.25000000E 01
                    0.25470497E 05
 0.30218894E 01-0.21737249E-02 0.37542203E-05-0.29947200E-08
 0.90777547E-12 0.29137190E 05
 0.41565016E 01-0.17244334E-02 0.56982316E-05-0.45930044E-08
 0.14233654E-11-0.30288770E 05
 0.38234708E 01-0.11187229E-02 0.12466819E-05-0.21035896E-09
-0.52546551E-13 0.35852787E 04
 0.37189946E 01-0.25167288E-02 0.85837353E-05-0.82998716E-08
 0.27082180E-11-0.10576706E 04
 0.28460849E 01 0.41932116E-02-0.96119332E-05 0.95122662E-08
-0.33093421E-11-0.96725372E 03
 0.36916148E 01-0.13332552E-02 0.26503100E-05-0.97688341E-09
-0.99772234E-13-0.10628336E 04
.2514793700E 01-.112437910E-03.2964750600E-06-.324640490E-09
.1259546500E-12.5612776700E 05
.4146947600E 01-.411972370E-02.9692246700E-05-.786336390E-08
.22[illegible]7951200E-11.9744789400E 04
.2382117100E 01.1035055600E-01-.111676340E-04.6958316500E-08
-.187801920E-11.8722996400E 04
.3434456300E 01.2223429700E-02.6714897500E-05-.974277190E-08
.3721252300E-11.2864768500E 04
.3787133200E 01-.217095260E-02.5075733700E-05-.347377280E-08
.7721684100E-12-.143635080E 05
.2170100000E 01.1037811500E-01-.107339380E-04.6345917500E-08
-.162807010E-11-.483526020E 05
                                          Blank Card
                   -.239000000E 05
 0.25000000E 01
                    0.25470497E 05
 0.25372567E 01-0.18422190E-04-0.88017921E-08 0.59643621E-11
-0.55743608E-15 0.29230007E 05
 0.26707532E 01 0.30317115E-02-0.85351570E-06 0.11790853E-09
-0.61973568E-14-0.29888994E 05
 0.28895544E 01 0.99835061E-03-0.21879904E-06 0.19802785E-10
-0.38452940E-15 0.38811792E 04
 0.35976129E 01 0.78145603E-03-0.22386670E-06 0.42490159E-10
-0.33460204E-14-0.11927918E 04
 0.30436897E 01 0.61187110E-03-0.73993551E-08-0.20331907E-10
 0.24593791E-14-0.85491002E 03
 0.28545761E 01 0.15976316E-02-0.62566254E-06 0.11315849E-09
-0.76897070E-14-0.89017445E 03
.2442226100E 01.1227618700E-03-.849927190E-07.2140083000E-10
-.125110580E-14.5614082100E 05
.3152936000E 01.1405995500E-02-.570784620E-06.1062820900E-09
-.737207830E-14.9852204800E 04
.4626547900E 01.3021680700E-02-.121560140E-05.2285595200E-09
-.158497010E-13.8535664500E 04
.4613921900E 01.2638663900E-02-.109485410E-05.2081842500E-09
-.146543910E-13 .2340378800E 04
.2951151900E 01.1552556700E-02-.619114110E-06.1135033600E-09
-.778827320E-14-.142318270E 05
.4412926600E 01.3192289600E-02-.129782300E-05.2414744600E-09
-.167429860E-13-.489440430E 05
                                          Blank Card
                   -.239000000E 05
 52097.7   59556.6   -57797.9  9312.5
 113024.6  21600.    19490.    8007.5     -26415.7  -94051.8   -59670
```

In CHEMIE, the INPUT/OUTPUT STATEMENTS are

```
      READ(5,600)(CW(J),J=1,ISP)
      WRITE(6,700)(CW(J),J=1,ISP)
      READ(5,601)(AU(K),K=1,IRE)
      WRITE(6,701)(AU(K),K=1,IRE)
      READ(5,601)(CU(K),K=1,IRE)
      WRITE(6,701)(CU(K),K=1,IRE)
      READ(5,602)(E(K) ,K=1,IRE)
      WRITE(6,702)(E(K) ,K=1,IRE)
      READ(5,602)(D(K) ,K=1,IRE)
      WRITE(6,702)(D(K) ,K=1,IRE)
      WRITE(6,703)
      READ(5,605) ((GNUF(J,K),J=1,ISP),K=1,IRE)
      WRITE(6,705) GNUF
      READ(5,605) ((GNUB(J,K),J=1,ISP),K=1,IRE)
      WRITE(6,705) GNUB
  605 FORMAT(7F10.0)
  705 FORMAT(2X,7F12.5)
      DO 5 K=1,IRE
    5 READ(5,606) AF(K),BF(K),AB(K),BB(K)
  606 FORMAT(4F10.0)






      READ(5,606) EN
```

Data are

```
 1.008     16.       18.016    17.008    32.       2.016     28.016        CW
14.008     30.008    44.016    46.008    28.011    44.011    142.286       CW
.72000E 15.33000E 13.62000E 14.77000E 13.31000E 16                         A
.54000E 18.47500E 17.35600E 19.39900E 21.10000E 16                         A
.54000E 22.71000E 13.32000E 10.15500E 14.18000E 11                         A
.26000E 13.20000E 09                                                       A
.55000E 14.14000E 13.32000E 15.83000E 14.70000E 18                         C
.15000E 17.61000E 15.10000E 15.90000E 15.18200E 14                         C
.20000E 17.47000E 15.13300E 11.70000E 14.58000E 11                         C
.14200E 15.10000E 10                                                       C
8504.   4026.   3019.   503.    55353.  62196.  113171. 59378.  75841.     E
30696.  37237.  3875.   19675.  0.      23651.  32105.  6914.              E
503.    3019.   10618.  9108.   0.      0.      0.      0.      0.         D
10769.  0.      13712.  3563.   37992.  0.      14090.  0.                 D
```

The GNUF are

1.				1.		
	1.				1.	
			1.		1.	
			2.			
					1.	
		1.				
						1.
				1.		
	1.					
		1.				
			1.			
			1.			
				1.		
	1.					
	1.					
1.	1.					
				1.		
	1.					
	2.					
				5.		
						1.

The GNUB are

	1.		1.			
1.			1.			
1.		1.				
	1.	1.				
2.						
1.			1.			
2.						
	2.					
	1.					
1.						
	1.					1.
	1.					
	1.					
1.						
					1.	
				1.		
1.						
1.						
	1.					1.
	1.					
			1.			
	1.					
		1.				
					11.	
				10.		

The AF, BF, AB, BB are

	1.		1.
	1.		1.
	1.		1.
	1.0		1.0
	1.	-1.	2.
	1.		2.
-.5	1.		2.
-1.	1.		2.
-1.5	1.		2.
	1.		2.
-1.	1.		2.
	1.		1.
1.	1.	1.	1.
	1.		1.
.5	1.	.5	1.
	1.		1.

This card all zeros

EN is

10.

SECTION III

LISTING OF PROGRAM

A listing of the program and data input are presented in this section

```
C     MAIN PROGRAM RRR00034
C
C     READ IN INTIAL PROFILES (VELOCITY,TEMPERATURE AND CONCENTRATIONS)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION DID(14),DES(14)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /TTT/ YOEI,YOEO
      COMMON /TGSK/ H(14)
      COMMON /SAX/ ZX,UM
      COMMON /UPSET/ A(51),B(51),C(51),D(14,51),V(14,51),ALP(51),BAK,A
     1SKA,BUK,PISK,IKS,IK,IA,KQ,KOR
      COMMON /SU/ DELX
      COMMON /SIG/ PA(14,14),PT(14),W(14,51)
      COMMON /SYLT/ E(14,51)
      COMMON /YYY/ IZE
      COMMON /CEN/ KRISE
      COMMON /SA/ AREX
      COMMON /SSS/ IAP
      COMMON /VVV/ YO(51)
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON /YP/ YEI(14),YEO(14)
      COMMON / RRR/ TO(51)
      COMMON /XXX/ TAU
      COMMON /UUU/ ZZ(51)
      KQ +VE INDICATES REGIME 2 HAS BEEN REACHED
      DATA NILS/51/,KRIS,JA,IT/-10,10,1/,KRYS,KRAS/-10,20/
      DATA Z/0.0/,KZ/500/,KRN/50/,KRI/10/,KILLE/10/,KUN/0/
      DATA KTELL/3/,CN/1.0D0/
      ISP=14
      IRE=17
      IMU=11
      TAU=.4D-3
      IZE=0
      KAN=-10
      KUM=0
      KYS=50
      KRISE=-10
      KQ=-10
      ZX=0.0
      CALL THERMO (KRIS,JA,IT)
```

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```
      IJ=1
      KRAS=20                                                           B  29
      KRYS=-11                                                          B  30
      CALL CHEMIF (KRYS,KRAS,IJ)                                        B  31
      WRITE (6,390)                                                     B  32
      CALL INIT                                                         B  33
      NINA=NNN                                                          B  34
      DELX=.00001
      RUP=DELX/(DPSI**2)
      ZMAX=.7
      AREX=DELX                                                         B  37
      KK1=1                                                             B  38
      KK2=NNN                                                           B  39
      NU=-10                                                            B  40
      CALL SPECIE (KK1,KK2,NU)                                          B  41
      JA=-10                                                            B  42
      KRIS=100                                                          B  43
      DO 20 I=1,NNN                                                     B  44
      UPR(I)=U(I)                                                       B  45
      IT=I                                                              B  46
      CALL THERMO (KRIS,JA,IT)                                          B  47
      HSI=0.0                                                           B  48
      DO 10 J=1,ISP                                                     B  49
      YPR(J,I)=Y(J,I)
   10 HSI=HSI+X(J,I)*H(J)                                               B  51
      HST(I)=HSI*1800./CM(I)                                            B  52
      HT(I)=(U(I)**2)/(2.*32.17*778.16)+HST(I)                          B  53
      TPR(I)=S(I)                                                       B  54
   20 HTPR(I)=HT(I)                                                     B  55
      HEI=HT(1)                                                         B  56
      HED=HT(NNN)                                                       B  57
      NLOW=1                                                            B  58
      NHIGH=NNN-1                                                       B  60
      CALL TRANSP(NLOW,NHIGH)
      IN=0
      CALL INTEG (NLOW,NHIGH,IN)                                        B  62
      WRITE (6,370) NNN                                                 B  63
      WRITE (6,380) (I,R(I),PSI(I),U(I),T(I),S(I),CM(I),Y(6,I),I=1,NNN) B  64
      WRITE (6,380) (I,R(I),PSI(I),HT(I),HST(I),HTPR(I),X(6,I),X(3,I),I=B  65
     11,NNN)                                                            B  66
   30 CONTINUE                                                          B  67
      DUPX=AREX                                                         B  68
      DELX=AREX                                                         B  69
                                                                        B  70
```

```
 40     Z=Z+DELX                                                                    B  71
        IF (Z.GT.ZMAX) GO TO 310                                                    B  72
        ZX=Z*12.                                                                    B  73
        KUN=KUN+1                                                                   B  74
        KUSK=0                                                                      B  75
        NEVU=NEU                                                                    B  76
        NEVL=NEL                                                                    B  77
        IA=NNN-1
        NEU=IA-4
        NEVU=NEU
        IK=NEL-4                                                                    B  79
        IF (IK.LE.1) IK=1                                                           B  80
        IKS=(IA-IK)+1                                                               B  81
        IKU=IKS-1                                                                   B  82
        RUP=DELX/(DPSI**2)                                                          B  83
        IF(IA.GE.(NILS-1)) GO TO 50
        GO TO 60                                                                    B  85
    50 CONTINUE
        KUN=0
        KUM=0
        CALL CHANGE(RUP)
        Z=ZX/12.
        IK=1
        IA=NNN-1
        NEU=IA-4
        IF (IK.LE.1) IK=1                                                           B  89
        IKS=(IA-IK)+1                                                               B  90
        NINA=NNN
        WRITE (6,370) NNN                                                           B  91
        WRITE (6,380) (I,R(I),PSI(I),U(I),T(I),S(I),CM(I),Y(6,I),I=1,NNN)           B  92
 60     KUSK=KUSK+1                                                                 B  93
        UEO=U(NNN)
        CALL SETUP (RUP)                                                            B  94
        CALL GAUSS                                                                  B  95
        KRYS=-11                                                                    B  96
        KRAS=5                                                                      B  97
        IJ=NNN
        CALL CHEMIE(KRYS,KRAS,IJ)
        DO 400 J=1,ISP
   400 E(J,NNN)=W(J,NNN)/U(NNN)
        DO 401 J=1,ISP
   401 Y(J,NNN)=DELX*E(J,NNN)+YPR(J,NNN)
        KK1=NNN
```

```
      KK2=NNN
      NU=10
      CALL SPECIE(KK1,KK2,NU)
      DO 402 J=1,ISP
  402 YEO(J)=Y(J,NNN)
      CMO=CM(NNN)
      JA=-10
      KRIS=10
      IT=NNN
      HST(NNN)=HT(NNN)-(U(NNN)**2)/(2.*32.17*778.76)
      CALL THERMO(KRIS,JA,IT)
      TEO=S(NNN)
      NU=0
      CALL SPECIE(KK1,KK2,NU)
      RHUO=ROU(NNN)
      DO 110 I=IK,IA                                                    B  99
      IF (KQ.GT.0) GO TO 70                                             B 100
      IF (I.LT.IK)  GO TO 90
   70 IF(I.GT.IA) GO TO 90
      IJ=I                                                              B 103
      CALL CHEMIE (KRYS,KRAS,IJ)                                        B 104
      DO 80 J=1,ISP
   80 E(J,I)=.5*(U(I)+UPR(I))*W(J,I)/(U(I)*UPR(I))                      B 1
      GO TO 110                                                         B 1
   90 DO 100 J=1,ISP
      E(J,I)=0.0                                                        B 109
  100 W(J,I)=0.0                                                        B 110
  110 CONTINUE                                                          B 111
      CALL SETYP (RUP)                                                  B 112
      CALL GAUSS                                                        B 113
      IF (KRISE.GT.0) GO TO 320                                         B 114
      CALL SETHP (RUP)                                                  B 115
      CALL GAUSS                                                        B 116
      KK1=IK                                                            B 117
      KK2=IA                                                            B 118
      JA=-10                                                            B 119
      KRIS=10                                                           B 120
      DO 120 I=IK,IA                                                    B 121
      IT=I                                                              B 122
      CALL THERMO (KRIS,JA,IT)                                          B 123
  120 CONTINUE                                                          B 124
      NU=0                                                              B 125
      CALL SPECIE (KK1,KK2,NU)                                          B 126
```

```
 130  NLOW=IK                                                         B 127
      NHIGH=IA                                                        B 128
      IN=+10                                                          B 129
      CALL TRANSP(NLOW,NHIGH)
      CALL INTEG (NLOW,NHIGH,IN)                                      B 130
      IF(KUN.EQ.50) KAN=10
      IF(KAN.LT.0) GO TO 623
      CALL PRINT (KUSK,KUN)                                           B 131
      KAN=-10
  623 CONTINUE
      UEO=U(NNN)
      CALL SETUP (RUP)                                                B 132
      CALL GAUSS                                                      B 133
      KRAS=0                                                          B 134
      KUSK=KUSK+1                                                     B 135
      DAD=(S(NNN)-TPR(NNN))/1.8
      T(NNN)=.5*(T(NNN)+TPR(NNN)/1.8)
      DO 403 J=1,ISP
      DID(J)=Y(J,NNN)-YPR(J,NNN)
  403 Y(J,NNN)=.5*(Y(J,NNN)+YPR(J,NNN))
      IJ=NNN
      CALL CHEMIE(KRYS,KRAS,IJ)
      DO 404 KI=1,ISP
      SUM=0.
      DO 405 J=1,ISP
      DES(J)=DID(J)*PA(J,KI)
  405 SUM=SUM+DES(J)
      BA=W(KI,NNN)/U(NNN)*2.
      BE=(DAD*PT(KI)+SUM)/U(NNN)
      E(KI,NNN)=.5*(BA+BE)
  404 CONTINUE
      DO 406 J=1,ISP
  406 Y(J,NNN)=DELX*E(J,NNN)+YPR(J,NNN)
      KK1=NNN
      KK2=NNN
      NU=10
      CALL SPECIE(KK1,KK2,NU)
      DO 407 J=1,ISP
  407 YEO(J)=Y(J,NNN)
      CMO=CM(NNN)
      JA=-10
      KRIS=10
      IT=NNN
```

```
      HST(NNN)=HT(NNN)-(U(NNN)**2)/(2.*32.17*778.76)
      CALL THERMO(KRIS,JA,IT)
      TEO=S(NNN)
      NU=0
      CALL SPECIE(KK1,KK2,NU)
      RHUO=ROU(NNN)
      DO 220 I=IK,IA                                              B 136
      IF (KO.GT.0) GO TO 140                                      B 137
      IF (I.LT.IK)  GO TO 200
  140 IF(I.GT.IA) GO TO 200
      DAD=(S(I)-TPR(I))/1.8
      T(I)=.5*(T(I)+TPR(I)/1.8)                                   B 141
      DO 150 J=1,ISP
      DID(J)=Y(J,I)-YPR(J,I)                                      B 143
  150 Y(J,I)=.5*(Y(J,I)+YPR(J,I))                                 B 144
      IJ=I                                                        B 145
      CALL CHEMIE (KRYS,KRAS,IJ)                                  B 146
      DO 190 KI=1,ISP
      SUM=0.0                                                     B 148
      DO 170 J=1,ISP
      IF (DABS(PA(J,KI)).GT.0.1D-30) GO TO 160                    B 150
      DES(J)=0.0                                                  B 151
      GO TO 170                                                   B 152
  160 DES(J)=DID(J)*PA(J,KI)                                      B 153
  170 SUM=SUM+DES(J)                                              B 154
      BA=(U(I)+UPR(I))*W(KI,I)/(U(I)*UPR(I))                      B 155
      BE=(DAD*PT(KI)+SUM)/U(I)                                    B 156
  180 E(KI,I)=.5*(BA+BE)                                          B 163
  190 CONTINUE                                                    B 164
      GO TO 220                                                   B 165
  200 DO 210 J=1,ISP
  210 E(J,I)=0.0                                                  B 167
  220 CONTINUE                                                    B 168
      CALL SETYP (RUP)                                            B 169
      CALL GAUSS                                                  B 170
      IF (KRISE.GT.0) GO TO 320                                   B 171
      CALL SETHP (RUP)                                            B 172
      CALL GAUSS                                                  B 173
      DO 230 I=IK,IA                                              B 174
      IT=I                                                        B 175
      CALL THERMO (KRIS,JA,IT)                                    B 176
  230 CONTINUE                                                    B 177
      NU=0                                                        B 178
```

```
      KK1=IK
      KK2=IA
      CALL SPECIE (KK1,KK2,NU)                                          B 179
      IF (KUSK.EQ.3) GO TO 240                                         BCH180
      GO TO 130                                                         B 181
  240 CONTINUE                                                          B 182
      IN=0                                                              B 184
      IF(IAP.LT.IA) GO TO 280
      NEU=IA-3
      IA=NNN
      NNN=NNN+1
      IF(NNN.GT.NILS) GO TO 50
      PSI(NNN)=PSI(NNN-1)+DPSI
      U(NNN)=U(NNN-1)
      UPR(NNN)=UPR(NNN-1)
      S(NNN)=S(NNN-1)
      T(NNN)=S(NNN)/1.8
      TPR(NNN)=TPR(NNN-1)
      DO 408 J=1,ISP
      Y(J,NNN)=Y(J,NNN-1)
      X(J,NNN)=X(J,NNN-1)
  408 YPR(J,NNN)=YPR(J,NNN-1)
      YO(NNN)=YO(NNN-1)
      TO(NNN)=TO(NNN-1)
      HT(NNN)=HT(NNN-1)
      HST(NNN)=HST(NNN-1)
      ZZ(NNN)=ZZ(NNN-1)
      ROU(NNN)=ROU(NNN-1)
      NLOW=IK
      NHIGH=NNN-1
      CALL TRANSP(NLOW,NHIGH)
      CALL INTEG(NLOW,NHIGH,IN)
  270 CONTINUE
  280 CONTINUE                                                          B 198
      IK=NEL-4                                                          B 199
      IF (IK.LE.1) IK=1                                                 B 200
      IKS=(IA-IK)+1                                                     B 201
      NLOW=IK                                                           B 202
      NHIGH=IA                                                          B 203
      CALL TRANSP(NLOW,NHIGH)
      CALL INTEG (NLOW,NHIGH,IN)                                        B 204
      DO 300 I=IK,NNN
      UPR(I)=U(I)                                                       B 206
```

```
          TPR(I)=S(I)                                                    B 207
          HTPR(I)=HT(I)                                                  B 208
          DO 290 J=1,ISP
  290     YPR(J,I)=Y(J,I)                                                B 210
  300     CONTINUE                                                       B 211
          KUM=KUM+1
          IF(KUM.NE.KYS) GO TO 624
          KUM=0
          IF(KUN.LT.100) GO TO 624
          CALL PRINT (KUSK,KUN)                                          B 212
      624 CONTINUE
          IF(KUN.EQ.2) GO TO 71
          IF(KUN.EQ.4) GO TO 72
          IF(KUN.LT.100) GO TO 73
          IF(KUN.GE.100) GO TO 74
          GO TO 3C                                                       B 213
  310     STOP                                                           B 214
       71 CONTINUE
          DELX=.00001
          GO TO 75
       72 CONTINUE
          DELX=.00001
          GO TO 75
       73 CONTINUE
          DELX=.00001
          GO TO 75
       74 CONTINUE
          DELX=.00001
       75 CONTINUE
          RUP=DELX/(DPSI**2)
          AREX=DELX
          GO TO 30
  320     KRISE=-10                                                      B 215
          Z=Z-DELX                                                       B 216
          DELX=DELX/2.
          KUN=KUN-1                                                      B 219
          NEL=NEVL                                                       B 220
          NEU=NEVU                                                       B 221
          GO TO 40                                                       B 223
C                                                                        B 224
  330     FORMAT (2X,4(2X,I5),14H SJEKK FOR NEU,/)                       B 225
  340     FORMAT (2X,2(2X,I4),6(2X,D14.7))                               B 226
  350     FORMAT (2X,7(2X,D14.7))                                        B 227
```

```
 360  FORMAT (//,2X,13HSTEP DECREASE,3(2X,D20.10),//)                 B 228
 380  FORMAT (2X,I4,7D18.7)                                           B 230
 370  FORMAT ('1',2X,4HNNN=,I4,////)
 390  FORMAT ('1')
      END                                                             B 232-
      SUBROUTINE SPECIE (KK1,KK2,NU)                                  C   1
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION G(14),CW(14)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU                        C   6
      COMMON/ZZZ/ISP,IRE,IMU
      DATA P/1.0D0/                                                 C   7
      DATA CW/1.008,16.0,18.016,17.008,32.0,2.016,28.016,14.008,30.008,
     1 44.016,46.008,28.011,44.011,142.286/
      DO 40 I=KK1,KK2                                                 C   9
      IF (NU.EQ.0) GO TO 30                                           C  10
      CM(I)=0.0                                                       C  11
      GM=0.0                                                          C  12
      DO 10 J=1,ISP
      G(J)=Y(J,I)/CW(J)                                               C  14
  10  GM=GM+G(J)                                                      C  15
      DO 20 J=1,ISP
      X(J,I)=G(J)/GM                                                  C  17
  20  CM(I)=CM(I)+X(J,I)*CW(J)                                        C  18
      IF (NU.EQ.10) GO TO 40                                          C  19
  30  CONTINUE                                                        C  20
      RM=1545.3/CM(I)                                                 C  21
      RO=P*2116.2/(RM*T(I)*1.8)                                       C  22
      ROU(I)=RO*U(I)                                                  C  23
  40  CONTINUE                                                        C  24
      RETURN                                                          C  25
      END                                                             C  26-
      SUBROUTINE THERMO (KRIS,JA,IT)                                  D   1
C     THERMODYNAMIC SUBROUTINE,BASED ON NASA SP-3001                  D   2
C     REFERENCE TEMPERATURE 298.15 DEG. K                             D   3
C     SPECIFSIH,O,H2O,OH,O2,H2,N2                                     D   4
C     FRYS -VE : IMPLIES FROZEN FLOW,HENCE SENS(J)NOT ZERO            D   5
C     JA   +VE : READ IN CONSTANTS                                    D   6
C     JA   -VE : CALCULATE ENTHALPIES                                 D   7
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(6,14),B(6,14),SENS(14)
```

```
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUD,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU                          D  12
      COMMON/ZZZ/ISP,IRE,IMO
      COMMON /TOSK/ H(14)
      M=IT                                                              D  14
      IF (JA) 10,10,180                                                 D  15
   10 CONTINUE                                                          D  16
      IF (KRIS.EQ.+100) GO TO 100                                       D  17
      NR=0                                                              D  18
      TP=S(M)                                                           D  19
      T(M)=TP/1.8                                                       D  20
      TO=TP                                                             D  21
   20 CONTINUE                                                          D  22
      HAS=0.0                                                           D  23
      GO TO 100                                                         D  24
   30 CONTINUE                                                          D  25
      DO 40 J=1,ISP
   40 HAS=HAS+X(J,M)*H(J)                                               D  27
      HTS=HAS*1800./CM(M)                                               D  28
      NR=NR+1                                                           D  29
      IF (NR.GE.20) GO TO 90                                            D  30
      CHH=HST(M)-HTS                                                    D  31
      CHK=DABS(CHH/HST(M))                                              D  32
      IF (CHK.LE.0.001) GO TO 90                                        D  33
      IF (NR.GE.2) GO TO 80                                             D  34
      TA=TP                                                             D  35
      FA=CHH                                                            D  36
      IF (CHH) 60,90,50                                                 D  37
   50 TP=TP+1.                                                          D  38
      GO TO 70                                                          D  39
   60 TP=TP-1.                                                          D  40
   70 T(M)=TP/1.8                                                       D  41
      GO TO 20                                                          D  42
   80 TB=TP                                                             D  43
      FB=CHH                                                            D  44
      IF ((FB-FA).EQ.0.0) GO TO 200                                     D  45
      TP=TA-FA*((TB-TA)/(FB-FA))                                        D  46
      T(M)=TP/1.8                                                       D  47
      FA=FB                                                             D  48
      TA=TB                                                             D  49
      GO TO 20                                                          D  50
```

```
90     CONTINUE                                                            D  51
       S(M)=T(M)*1.8                                                       D  52
       GO TO 170                                                           D  57
100    CONTINUE                                                            D  58
       G=1.98726                                                           D  59
       DO 160 J=1,ISP
       IF (T(M)-1000.) 110,110,120                                         D  61
110    HA=A(1,J)+(A(2,J)/2.+(A(3,J)/3.+(A(4,J)/4.+(A(5,J)/5.)*T(M))*T(M))  D  62
      1*T(M))*T(M)+A(6,J)/T(M)                                             D  63
       GO TO 130                                                           D  64
120    HA=B(1,J)+(B(2,J)/2.+(B(3,J)/3.+(B(4,J)/4.+(B(5,J)/5.)*T(M))*T(M))  D  65
      1*T(M))*T(M)+B(6,J)/T(M)                                             D  66
130    IF (KRIS) 140,140,150                                               D  67
140    CONTINUE                                                            D  68
       H(J)=(HA*G*T(M)-SENS(J))/1000.                                      D  69
       GO TO 160                                                           D  70
150    H(J)=HA*G*T(M)/1000.                                                D  71
160    CONTINUE                                                            D  72
       IF (KRIS.EQ.+100) GO TO 170                                         D  73
       GO TO 30                                                            D  74
170    CONTINUE                                                            D  75
       RETURN                                                              D  76
180    READ (5,260) ((A(K,J),K=1,6),J=1,ISP)
       DO 190 J=1,ISP
       READ (5,260) (B(K,J),K=1,6)                                         D  80
       WRITE (6,280) (B(K,J),K=1,6)                                        D  81
190    CONTINUE                                                            D  82
       READ (5,270) (SENS(J),J=1,ISP)
       GO TO 170                                                           D  84
200    WRITE (6,210) M,R(M),PSI(M),HST(M),HTS,FA,FB,TP,T(M)                D  85
       GO TO 90                                                            D  86
C                                                                          D  87
210    FORMAT (///,2X,I4,8(2X,E13.5),1X,4HTHFR,///)                        D  88
220    FORMAT (/,2(2X,I5),6(2X,E15.8))                                     D  89
230    FORMAT (2X,I5,4(2X,E15.8))                                          D  90
240    FORMAT (2X,I5,7(2X,E15.8))                                          D  91
250    FORMAT (2X,I5,7(2X,E15.8),/)                                        D  92
260    FORMAT (4D15.8,/2D15.8)                                             D  93
270    FORMAT (7D10.0)                                                     D  94
280    FORMAT (/////,1X,6E20.8,//////)                                     D  95
       END                                                                 D  96-
       SUBROUTINE INIT
       IMPLICIT REAL*8(A-H,O-Z)
```

```
      DIMENSION UE(51),SE(51),YE(14,51),PS(51)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /TTT/ YOEI,YOEO
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON / RRR/ TO(51)
      COMMON /YP/ YEI(14),YEO(14)
      COMMON /UUU/ ZZ(51)
      COMMON /VVV/ YO(51)
      READ(5,100) NNN
      READ(5,101)(UE(L),SE(L),R(L),L=1,NNN)
      READ(5,102)((YE(J,I),J=1,ISP),I=1,NNN)
      DO 40 L=1,NNN
      S(L)=SE(L)
      T(L)=S(L)/1.8
      U(L)=UE(L)
      DO 30 J=1,ISP
   30 Y(J,L)=YE(J,L)
   40 CONTINUE
      KK1=1
      KK2=NNN
      NU=-10
      CALL SPECIE (KK1,KK2,NU)
      PS(1)=0.
      FRO=0.
      DSI=0.
      DO 50 L=1,NNN
      IF((L-2).LT.0) GO TO 50
      DELR=(R(L)-R(L-1))/12.
      FRI=ROU(L)*R(L)/12.
      DP=DELR*(FRO+FRI)
      FRO=FRI
      DSI=DSI+DP
      PS(L)=DSQRT(DSI)
   50 CONTINUE
      UEI=U(1)
      UEO=U(NNN)
      TEI=S(1)
      TEO=S(NNN)
      CMEI=CM(1)
      CMO=CM(NNN)
```

```
      DO 60 J=1,ISP
      YEI(J)=Y(J,1)
   60 YEO(J)=Y(J,NNN)
      DPSI=PS(NNN)/(NNN-1)
      RHUE=ROU(1)
      RHUO=ROU(NNN)
      PSI(1)=0.
      DO 2 J=2,NNN
    2 PSI(J)=PSI(J-1)+DPSI
      NM1=NNN-1
      DO 3 J=2,NM1
      DO 4 K=1,NNN
      DIF=PSI(J)-PS(K)
      IF(DIF) 5,6,4
    6 U(J)=UE(K)
      S(J)=SE(K)
      T(J)=S(J)/1.8
      DO 8 L=1,ISP
    8 Y(L,J)=YE(L,K)
      GO TO 3
    5 RAT=(PSI(J)-PS(K-1))/(PS(K)-PS(K-1))
      U(J)=UE(K-1)+RAT*(UE(K)-UE(K-1))
      S(J)=SE(K-1)+RAT*(SE(K)-SE(K-1))
      T(J)=S(J)/1.8
      DO 9 L=1,ISP
    9 Y(L,J)=YE(L,K-1)+RAT*(YE(L,K)-YE(L,K-1))
      GO TO 3
    4 CONTINUE
    3 CONTINUE
      PSI(NNN)=PS(NNN)
      NEL=1
      NEU=22
      DO 11 J=1,NNN
   11 YO(J)=Y(ISP,J)
      DO 12 J=NEL,NNN
   12 ZZ(J)=0.
      DO 14 J=1,NNN
   14 TO(J)=0.
      YOEI=Y(ISP,1)
      YOEO=Y(ISP,NNN)
      RETURN
  100 FORMAT(I5)
  101 FORMAT(3F10.0)
```

```
  102 FORMAT(7D10.0)
      END
      SUBROUTINE TRANSP(NLOW,NHIGH)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /SAX/ ZX,UM
      DATA RJ /.2/
      COEFF=.036/RJ
      L=NLOW
      LL=NHIGH+1
      SUM=0.
      DO 1 K=L,LL
      ARG=DABS((ROU(LL)-ROU(K))/ROU(K))*PSI(K)
    1 SUM=SUM+ARG
      SUM=SUM*DPSI
      UM=SUM*COEFF
      RETURN
      END
      SUBROUTINE INTEG (NLOW,NHIGH,IN)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /SAX/ ZX,UM
C     INTEGRATION ROUTINE BACK TO PHYSICAL PLANE
C     IF IN GT.THAN 0.0 A IS AVERAGED
C     IF IN EQ.TO 0.0 A IS BASED ON PAST TIME ROW.
      INIT=1
      L=NLOW
      LL=NHIGH+1
      DO 60 K=L,LL
      IF (INIT-2) 10,30,30
   10 DM=PSI(K)
      IF (DM.EQ.0.0) GO TO 20
      IK=K
      FI=PSI(K)/ROU(K)
      B=FI*DM
      R(K)=(DSQRT(B))*12.
      RR=(R(K)/12.)**2
```

```
      SP=UM*ROU(K)*RR/PSI(K)
      FO=FI
      INIT=10
      GO TO 40
   20 R(K)=0.0
      B=0.0
      FO=0.0
      SP=0.0
      INIT=10
      GO TO 40
   30 IK=K
      FI=PSI(K)/ROU(K)
      BR=(FO+FI)*DPSI
      B=B+BR
      R(K)=(DSQRT(B))*12.
      RR=(R(K)/12.)**2
      IF (PSI(K).EQ.0.0) GO TO 70
      SP=UM*ROU(K)*RR/PSI(K)
      FO=FI
   40 IF (IN.EQ.0) GO TO 50
      AP(K)=.5*(SP+APR(K))
      GO TO 60
   50 APR(K)=SP
      AP(K)=SP
   60 CONTINUE
      RETURN
   70 WRITE (6,80) K,L,LL,ZX,U(K)
      STOP
C
   80 FORMAT (//,11HINTEG. STOP,3X,3(2X,I4),2(3X,F15.8))
      END
      SUBROUTINE SETUP (RUP)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /UPSET/ A(51),B(51),C(51),D(14,51),V(14,51),ALP(51),RAK,A
     1SKA,RUK,PISK,IKS,IK,IA,KO,KOR
      COMMON /SAX/ ZX,UM
      Q=RUP
      I=IK-1
      DO 50 K=1,IKS
```

```
      I=I+1
      IF (K.EQ.1) GO TO 10
      IF (K.EQ.IKS) GO TO 40
      A(I)=Q*(AP(I)-.25*AP(I+1)+.25*AP(I-1))
      B(I)=2.*(PSI(I)+AP(I)*Q)
      C(I)=Q*(AP(I)+.25*AP(I+1)-.25*AP(I-1))
      BAK=2.*(PSI(I)-AP(I)*Q)
      D(1,I)=A(I)*UPR(I-1)+BAK*UPR(I)+C(I)*UPR(I+1)
      ALP(I)=B(I)-A(I)*C(I-1)/ALP(I-1)
      V(1,I)=D(1,I)+A(I)*V(1,I-1)/ALP(I-1)
      GO TO 50
   10 A(I)=0.0
      IF (IK.EQ.1) GO TO 20
      B(I)=2.*(PSI(I)+AP(I)*Q)
      C(I)=Q*(AP(I)+.25*AP(I+1)-.25*AP(I-1))
      ASKA=Q*(AP(I)-.25*AP(I+1)+.25*AP(I-1))
      BAK=2.*(PSI(I)-AP(I)*Q)
      D(1,I)=2.*ASKA*UEI+BAK*UPR(I)+C(I)*UPR(I+1)
      GO TO 30
   20 B(I)=1.+2.*UM*Q
      C(I)=2.*UM*Q
      D(1,I)=(1.-2.*UM*Q)*UPR(I)+C(I)*UPR(I+1)
   30 ALP(I)=B(I)
      V(1,I)=D(1,I)
      GO TO 50
   40 C(I)=0.0
      A(I)=Q*(AP(I)-.25*AP(I+1)+.25*AP(I-1))
      B(I)=2.*(PSI(I)+AP(I)*Q)
      BUK=2.*(PSI(I)-AP(I)*Q)
      PISK=Q*(AP(I)+.25*AP(I+1)-.25*AP(I-1))
      D(1,I)=A(I)*UPR(I-1)+BUK*UPR(I)+2.*PISK*UEO
      ALP(I)=B(I)-A(I)*C(I-1)/ALP(I-1)
      V(1,I)=D(1,I)+A(I)*V(1,I-1)/ALP(I-1)
   50 CONTINUE
      DO 60 I=IK,IA
   60 CONTINUE
      KOR=-10
      RETURN
C
      END
      SUBROUTINE SETYP (RUP)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
```

```
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /UPSET/ A(51),B(51),C(51),D(14,51),V(14,51),ALP(51),BAK,A
     ISKA,BUK,PISK,IKS,IK,IA,KO,KOR
      COMMON /SYLT/ E(14,51)
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON /SU/ DELX
      COMMON /YP/ YEI(14),YEO(14)
      COMMON /SAX/ ZX,UM
      DATA CN/1.0D0/
      Q=RUP
      I=IK-1
      DO 100 K=1,IKS
      I=I+1
      IF (K.EQ.1) GO TO 20
      IF (K.EQ.IKS) GO TO 80
      A(I)=CN*A(I)
      B(I)=2.*(PSI(I)+AP(I)*Q*CN)
      C(I)=CN*C(I)
      BAK=2.*(PSI(I)-AP(I)*Q*CN)
      ALP(I)=B(I)-A(I)*C(I-1)/ALP(I-1)
      DAX=2.*PSI(I)*DELX
      DO 10 J=1,ISP
      D(J,I)=A(I)*YPR(J,I-1)+BAK*YPR(J,I)+C(I)*YPR(J,I+1)+E(J,I)*DAX
   10 V(J,I)=D(J,I)+A(I)*V(J,I-1)/ALP(I-1)
      GO TO 100
   20 A(I)=0.0
      IF (IK.EQ.1) GO TO 40
      B(I)=2.*(PSI(I)+AP(I)*Q*CN)
      C(I)=CN*C(I)
      ASKA=CN*ASKA
      BAK=2.*(PSI(I)-AP(I)*Q*CN)
      DAX=2.*PSI(I)*DELX
      DAX=2.*PSI(I)*DELX
      DO 30 J=1,ISP
   30 D(J,I)=2.*ASKA*YEI(J)+BAK*YPR(J,I)+C(I)*YPR(J,I+1)+E(J,I)*DAX
      GO TO 60
   40 B(I)=1.+2.*UM*CN*Q
      C(I)=2.*UM*CN*Q
      DO 50 J=1,ISP
   50 D(J,I)=(1.-2.*UM*CN*Q)*YPR(J,I)+C(I)*YPR(J,I+1)+E(J,I)*DELX
   60 ALP(I)=B(I)
```

```
      DO 70 J=1,ISP
70    V(J,I)=D(J,I)                                                  I 45
      GO TO 100                                                      I 46
80    C(I)=0.0                                                       I 47
      A(I)=CN*A(I)                                                   I 48
      B(I)=2.*(PSI(I)+AP(I)*Q*CN)                                    I 49
      BUK=2.*(PSI(I)-AP(I)*Q*CN)                                     I 50
      PISK=CN*PISK                                                   I 51
      ALP(I)=B(I)-A(I)*C(I-1)/ALP(I-1)                               I 52
      DAX=2.*PSI(I)*DELX                                             I 53
      DO 90 J=1,ISP
      D(J,I)=A(I)*YPR(J,I-1)+BUK*YPR(J,I)+   PISK*YEO(J)+E(J,I)*DAX  I 55
     1+PISK*YPR(J,IN)
90    V(J,I)=D(J,I)+A(I)*V(J,I-1)/ALP(I-1)                           I 56
100   CONTINUE                                                       I 57
      DO 110 I=IK,IA                                                 I 58
110   CONTINUE                                                       I 59
      KOR=0                                                          I 60
      RETURN                                                         I 61
C                                                                    I 62
      END                                                            I 63-
      SUBROUTINE SETHP (RUP)                                         J 1
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHOE,RHOO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEO                       J 5
      COMMON /UPSET/ A(51),B(51),C(51),D(14,51),V(14,51),ALP(51),BAK,A
     1SKA,BUK,PISK,IKS,IK,IA,KO,KOR
      COMMON /SAX/ ZX,UM                                             J 8
      DATA CN/1.000/
      Q=RUP                                                          J 9
      I=IK-1                                                         J 10
      DO 50 K=1,IKS                                                  J 11
      I=I+1                                                          J 12
      IF (K.EQ.1) GO TO 10                                           J 13
      IF (K.EQ.IKS) GO TO 40                                         J 14
      BAK=2.*(PSI(I)-AP(I)*Q*CN)                                     J 15
      D(1,I)=A(I)*HTPR(I-1)+BAK*HTPR(I)+C(I)*HTPR(I+1)               J 16
      V(1,I)=D(1,I)+A(I)*V(1,I-1)/ALP(I-1)                           J 17
      GO TO 50                                                       J 18
10    IF (IK.EQ.1) GO TO 20                                          J 19
      BAK=2.*(PSI(I)-AP(I)*Q*CN)                                     J 20
```

```
      ASKA=D*(AP(I)-.25*AP(I+1)+.25*AP(I-1))*CN
      D(1,I)=2.*ASKA*HEI+BAK*HTPR(I)+C(I)*HTPR(I+1)
      GO TO 30
20    D(1,I)=(1.-2.*UM*Q*CN)*HTPR(I)+C(I)*HTPR(I+1)
30    V(1,I)=D(1,I)
      GO TO 50
40    BUK=2.*(PSI(I)-AP(I)*Q*CN)
      PISK=D*(AP(I)+.25*AP(I+1)-.25*AP(I-1))*CN
      D(1,I)=A(I)*HTPR(I-1)+BUK*HTPR(I)+2.*PISK*HEO
      V(1,I)=D(1,I)+A(I)*V(1,I-1)/ALP(I-1)
50    CONTINUE
      DO 60 I=IK,IA
60    CONTINUE
      KOR=+10
      RETURN
C
      END
      SUBROUTINE GAUSS
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION G(14),CW(14)
      DIMENSION NE(3), NO(3)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /UPSET/ A(51),B(51),C(51),D(14,51),V(14,51),ALP(51),BAK,A
     1SKA,BUK,PISK,IKS,IK,IA,KO,KOR
      COMMON /SSS/ IAP
      COMMON /OOO/ ZZ(51)
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON /CEN/ KRISE
      DATA TOL/1.0D-04/
      DATA CW/1.008,16.0,18.016,17.008,32.0,2.016,28.016,14.008,30.008,
     1 44.016,46.008,28.011,44.011,142.286/
      IF(NO(3).LT.IA) GO TO 1
      WRITE(6,310) NO(1),NO(2),NO(3)
      NO(3)=0
    1 IB=IA+1
      KAS=-10
      KOS=-10
      IF (KOR) 10,70,170
10    DO 60 M=1,IKS
      IB=IB-1
```

```
      IF (M.EQ.1) GO TO 20                                    K  19
      U(IB)=(V(1,IB)+C(IB)*U(IB+1))/ALP(IB)                   K  20
      GO TO 30                                                K  21
20    U(IB)=V(1,IB)/ALP(IB)                                   K  22
30    CONTINUE                                                K  24
      IF (KOS.GT.0) GO TO 40                                  K  25
      IF (DABS(U(IB)-UEO)/UEO.GT.TOL) GO TO 50                K  26
40    CONTINUE                                                K  27
      IF (KAS.GT.0) GO TO 60                                  K  28
      IF ((DABS(U(IB)-UEI)/UEI).GT.TOL) GO TO 60              K  29
      KAS=+10                                                 K  30
      NE(I)=IB                                                K  31
      GO TO 60                                                K  32
50    NO(I)=IB                                                K  33
      KOS=+10                                                 K  34
60    CONTINUE                                                K  35
      IF (KAS.LT.0) NE(I)=IK                                  K  36
      GO TO 300                                               K  38
70    DO 160 M=1,IKS                                          K  39
      IB=IB-1                                                 K  40
      IF (M.EQ.1) GO TO 90                                    K  41
      DO 80 J=1,ISP
      Y(J,IB)=(V(J,IB)+C(IB)*Y(J,IB+1))/ALP(IB)               K  43
80    CONTINUE                                                K  44
      GO TO 110                                               K  45
90    DO 100 J=1,ISP
      Y(J,IB)=V(J,IB)/ALP(IB)                                 K  47
100   CONTINUE                                                K  48
110   CONTINUE                                                K  49
      CM(IB)=0.0                                              K  50
      GM=0.0                                                  K  51
      DO 120 J=1,ISP
      G(J)=Y(J,IB)/CW(J)                                      K  53
120   GM=GM+G(J)                                              K  54
      DO 130 J=1,ISP
      X(J,IB)=G(J)/GM                                         K  56
130   CM(IB)=CM(IB)+X(J,IB)*CW(J)                             K  57
      IF(M.EQ.1) GO TO 160
      IF (KOS.GT.0) GO TO 140                                 K  58
      IF (DABS(CM(IB)-CMO)/CMO.GT.TOL) GO TO 150              K  59
140   CONTINUE                                                K  60
      IF (KAS.GT.0) GO TO 160                                 K  61
      IF (DABS(CM(IB)-CMEI)/CMEI.GT.TOL) GO TO 160            K  62
```

```
      NE(2)=IB                                                          K  63
      KAS=+10                                                           K  64
      GO TO 160                                                         K  65
  150 NO(2)=IB                                                          K  66
      KOS=+10                                                           K  67
  160 CONTINUE                                                          K  68
      IF (KAS.LT.0) NE(2)=IK                                            K  69
      GO TO 300                                                         K  71
  170 DO 220 M=1,IKS                                                    K  72
      IB=IB-1                                                           K  73
      IF (M.EQ.1) GO TO 180                                             K  74
      HT(IB)=(V(1,IB)+C(IB)*HT(IB+1))/ALP(IB)                           K  75
      HST(IB)=HT(IB)-(U(IB)**2)/(2.*32.17*778.16)                       K  76
      GO TO 190                                                         K  77
  180 HT(IB)=V(1,IB)/ALP(IB)                                            K  78
      HST(IB)=HT(IB)-(U(IB)**2)/(2.*32.17*778.16)                       K  79
      GO TO 220                                                         K  80
  190 CONTINUE                                                          K  81
      IF (KOS.GT.0) GO TO 200                                           K  82
      IF(DABS((HT(IB)-HEO)/HEO).GT.TOL) GO TO 210
  200 CONTINUE                                                          K  84
      IF (KAS.GT.0) GO TO 220                                           K  85
      IF (DABS(HT(IB)-HEI)/HEI.GT.TOL) GO TO 220                        K  86
      KAS=+10                                                           K  87
      NE(3)=IB                                                          K  88
      GO TO 220                                                         K  89
  210 NO(3)=IB                                                          K  90
      KOS=+10                                                           K  91
  220 CONTINUE                                                          K  92
      IF (KAS.LT.0) NE(3)=IK                                            K  95
      IF (NE(1).EQ.1.OR.NE(2).EQ.1.OR.NE(3).EQ.1) KQ=+10                K  96
      IF (NE(1).LT.NE(2)) GO TO 230                                     K  97
      NU=NE(2)                                                          K  98
      GO TO 240                                                         K  99
  230 NU=NE(1)                                                          K 100
  240 IF (NU.LT.NE(3)) GO TO 250                                        K 101
      NFL=1
      GO TO 260                                                         K 103
  250 NFL=1
  260 IF (NO(1).GT.NO(2)) GO TO 270                                     K 105
      MU=NO(2)                                                          K 106
      GO TO 280                                                         K 107
  270 MU=NO(1)                                                          K 108
```

```
280   IF (MU.GT.NO(3)) GO TO 290                                K 109
      IAP=NO(3)
      GO TO 300                                                 K 111
290   IAP=MU
      IF (NEL.EQ.1) KO=+10                                      K 113
      MN=NEU+3-IA
      IF(IA.GT.0) GO TO 300
      I2=IA-4
      MNP1=MN+1
      DO 600 KK=1,MNP1
  600 ZZ(I0+MN)=ZX/12.
300   RETURN                                                    K 114
C                                                               K 115
310   FORMAT (2X,5HGAUSS,2X,3I10)                               K 116
320   FORMAT (2X,I4,4F22.10)                                    K 117
      END                                                       K 118-
      SUBROUTINE CHANGE(RUP)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),D(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU                  L   5
       COMMON/SAX/ ZX,UM
      COMMON / RRR/ TO(51)
      COMMON /UUU/ ZZ(51)
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON /SU/ DELX                                          L   6
      COMMON /VVV/ YO(51)
      COMMON /SA/ AREX                                          L   7
      PSA=PSI(NNN)
      NNN=(NNN-1)/2+1                                           L   9
      DPSI=PSA/(NNN-1)
      DAX=DELX*12.                                              L  11
      ZAX=ZX
      DX=(ZX/12.)-DELX                                          L  13
      AREX=DELX                                                 L  15
      RUP=DELX/(DPSI**2)
      DIX=DELX*12.                                              L  16
      DX=DX+DELX
      ZIX=DX*12.
      ZX=ZIX
      DO 40 MI=1,NNN                                            L  19
      IF ((MI-2).LT.0) GO TO 30                                 L  20
```

```
      MA=MA+2                                                          L  21
   10 PSI(MI)=PSI(MA)                                                  L  22
      AP(MI)=AP(MA)                                                    L  23
      APR(MI)=APR(MA)                                                  L  24
      R(MI)=R(MA)                                                      L  25
      U(MI)=U(MA)                                                      L  26
      UPR(MI)=UPR(MA)                                                  L  27
      HT(MI)=HT(MA)                                                    L  28
      HTPR(MI)=HTPR(MA)                                                L  29
      YO(MI)=YO(MA)
      TU(MI)=TU(MA)
      ZZ(MI)=ZZ(MA)
      S(MI)=S(MA)                                                      L  30
      T(MI)=T(MA)                                                      L  31
      TPR(MI)=TPR(MA)                                                  L  32
      DO 20 J=1,ISP
      Y(J,MI)=Y(J,MA)                                                  L  34
   20 YPR(J,MI)=YPR(J,MA)                                              L  35
      GO TO 40                                                         L  36
   30 MA=1                                                             L  37
      GO TO 10                                                         L  38
   40 CONTINUE                                                         L  39
      NIL=NEL/2+1                                                      L  40
      NIU=NEU/2+1                                                      L  41
      NEL=NIL                                                          L  42
      NEU=NIU                                                          L  43
      WRITE (6,50)                                                     L  44
      WRITE (6,60) NEL,NEU                                             L  45
      WRITE (6,70) ZAX,DAX,ZIX,DIX                                     L  46
      RETURN                                                           L  47
C                                                                      L  48
   50 FORMAT (///,2X,20HNR. OF POINTS HALVED)                          L  49
   60 FORMAT (2X,5HNEL= ,I5,5HNEU= ,I5)                                L  50
   70 FORMAT (2X,4HZAX=,F14.10,2X,4HDAX=,F14.10,2X,4HZIX=,F14.10,2X,4HDI L  51
     1X=,F14.10,///)                                                   L  52
      END                                                              L  53-
      SUBROUTINE PRINT (KUSK,KUN)                                      M   1
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AF(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU                         M   5
      COMMON /SAX/ ZX,UM                                               M   6
```

```
      COMMON /UPSET/ A(51),B(51),C(51),D(14,51),V(14,51),ALP(51),BAK,A
     1SKA,BUK,PISK,IKS,IK,IA,KO,KOR
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON /SU/ DELX                                                  M   9
      COMMON /SIG/ PA(14,14),PT(14),W(14,51)
      COMMON /SYLT/ E(14,51)
      Z=ZX/12.                                                          M  12
      WRITE (6,30) Z,ZX,DELX,DPSI,NEL,NEU,IKS,KUSK,KUN                  M  13
      DO 20 I=IK,IA                                                     M  14
      YTOT=0.0                                                          M  15
      DO 10 J=1,ISP
   10 YTOT=YTOT+Y(J,I)                                                  M  17
      WRITE (6,40) I,PSI(I),R(I),S(I),U(I),AP(I),APR(I),HT(I)           M  18
      WRITE (6,50) I,(Y(J,I),J=1,ISP)
      WRITE (6,50) I,(W(J,I),J=1,ISP)
      WRITE (6,50) I,(E(J,I),J=1,ISP)
      WRITE (6,60) I,YTOT,CM(I),ROU(I)                                  M  22
   20 CONTINUE                                                          M  23
      WRITE(6,60) KO,UM
      RETURN                                                            M  24
C                                                                       M  25
   30 FORMAT ('1',////,4(2X,F15.10),5(3X,I5),7H OUTPUT,///)
   40 FORMAT (/,2X,I4,7(2X,E14.7))                                      M  27
   50 FORMAT (2X,I4,7(2X,E14.7)/,6X,7(2X,E14.7))
   60 FORMAT (2X,I4,3(2X,E14.7))                                        M  29
      END                                                               M  30-
      SUBROUTINE CHEMIE (KRYS,KRAS,IJ)                                  N   1
C     SPECIE PRODUCTION SUBROUTINE -W/(RHO)*U - 1./FEET                 N   2
C     INPUT REQD. PRESSURE(ATM),AXIAL STEP SIZE(FT),NR. OF RADIAL MESH  N   3
C                 POINTS(NNN),TEMP(DEG.K) AND SPECIE MASS FRACTIONS     N   4
C     REACTIONS CONSIDERED:  H + O2 = OH + O          (1)               N   5
C                            O + H2 = OH + H          (2)               N   6
C                            H2+ OH =  H + H2O        (3)               N   7
C                              2OH =  O + H2O         (4)               N   8
C                            H2+ M  = 2H + M          (5)               N   9
C                            H2O+M  = OH + H + M      (6)               N  10
C                            OH +M  = O  + H + M      (7)               N  11
C                            O2 +M  = 2O + M          (8)               N  12
C                            H2 +O2 = OH + OH         (9)               N  13
C     FRYS = -VE:  FROZEN FLOW
C     FRYS = +VE:  FINITE RATE CHEMISTRY
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION CW(18), AU(22), CU(22), E(22), D(22), A(22)
```

```
      DIMENSION C(22), G(18)
      DIMENSION AF(22),BF(22),AB(22),BB(22)
      DIMENSION Z(18), F(22), B(22), FW(22), BW(22), CR(22)
      DIMENSION PRT(22),PK(18,22)
      DIMENSION GNUF(14,17), GNUB(14,17)
      COMMON R(51),S(51),U(51),Y(14,51),ROU(51),T(51),PSI(51)
      COMMON UPR(51),YPR(14,51),HST(51),HT(51),TPR(51),HTPR(51)
      COMMON CM(51),X(14,51),AP(51),APR(51),UEO,UEI,RHUE,RHUO,TEI,TEO
      COMMON HEI,HEO,CMEI,CMO,DPSI,NNN,NEL,NEU
      COMMON /SIG/ PA(14,14), PT(14), W(14,51)
      COMMON /UUU/ ZZ(51)
      COMMON/ZZZ/ISP,IRE,IMU
      COMMON /YYY/ IZE
      COMMON /SU/ DELX
      COMMON /SAX/ ZX,UM
      COMMON / RRR/ TO(51)
      COMMON /XXX/ TAU
      COMMON /VVV/ YO(51)
      KF=KRYS+KRAS
      P=1.00
      IF (KF.LT.0) GO TO 50
      CNV=453.5924/(30.4801**3)
      CNV2=CNV**2
      READ(5,600)(CW(J),J=1,ISP)
      WRITE(6,700)(CW(J),J=1,ISP)
      READ(5,601)(AU(K),K=1,IRE)
      WRITE(6,701)(AU(K),K=1,IRE)
      READ(5,601)(CU(K),K=1,IRE)
      WRITE(6,701)(CU(K),K=1,IRE)
      READ(5,602)(E(K) ,K=1,IRE)
      WRITE(6,702)(E(K) ,K=1,IRE)
      READ(5,602)(D(K) ,K=1,IRE)
      WRITE(6,702)(D(K) ,K=1,IRE)
      WRITE(6,703)
      READ(5,605) ((GNUF(J,K),J=1,ISP),K=1,IRE)
      WRITE(6,705) GNUF
      READ(5,605) ((GNUB(J,K),J=1,ISP),K=1,IRE)
      WRITE(6,705) GNUB
  605 FORMAT(7F10.0)
  705 FORMAT(2X,7F12.5)
      DO 5 K=1,IRE
    5 READ(5,606) AF(K),BF(K),AB(K),BB(K)
  606 FORMAT(4F10.0)
```

```
      READ(5,606) EN
      IMP=IMU+1
      DO 1 I=1,IRE
      A(I)=DLOG(AU(I)*CNV)
      IF(I.GT.4.AND.I.LT.IMP) GO TO 2
      C(I)=DLOG(CU(I)*CNV)
      GO TO 1
    2 C(I)=DLOG(CU(I)*CNV2)
    1 CONTINUE
      A(IRE)=DLOG(AU(IRE))
      C(IRE)=DLOG(CU(IRE))
      GO TO 20
   50 I=IJ
      IF (KRAS.EQ.0) GO TO 401
      TO(I)=TO(I)+.5*DELX*(1./U(I)+1./UPR(I))
  401 CONTINUE
      P=1.
      GM=0.0
      DO 10 J=1,ISP
      G(J)=Y(J,I)/CW(J)
   10 GM=GM+G(J)
      SM=0.0
      DO 11 J=1,ISP
      Z(J)=G(J)/GM
   11 SM=SM+Z(J)*CW(J)
      RM=1545.3/SM
      RO=P*2116.2/(RM*T(I)*1.8)
      DO 13 LK=1,IRE
      F(LK)=DEXP(A(LK)-E(LK)/T(I))
      B(LK)=DEXP(C(LK)-D(LK)/T(I))
   13 CONTINUE
      B(5)=B(5)/T(I)
      F(7)=F(7)/(T(I)**0.5)
      F(8)=F(8)/T(I)
      F(9)=F(9)/(T(I)**1.5)
      F(11)=F(11)/T(I)
      F(13)=F(13)*T(I)
      B(13)=B(13)*T(I)
      F(15)=F(15)*(T(I)**0.5)
      B(15)=B(15)*(T(I)**0.5)
      F(17)=F(17)*(P**0.3)*(T(I)/1111.0-0.5)
      FW(1)=F(1)*RO*G(1)*G(5)
      BW(1)=B(1)*RO*G(4)*G(2)
```

```
      FW(2)=F(2)*RO*G(6)*G(2)
      BW(2)=B(2)*RO*G(4)*G(1)
      FW(3)=F(3)*RO*G(6)*G(4)
      BW(3)=B(3)*RO*G(1)*G(3)
      FW(4)=F(4)*RO*G(4)*G(4)
      BW(4)=B(4)*RO*G(3)*G(2)
      FW(5)=F(5)*RO*G(6)*GM
      BW(5)=B(5)*RO*RO*G(1)*G(1)*GM
      FW(6)=F(6)*RO*G(3)*GM
      BW(6)=B(6)*RO*RO*G(4)*G(1)*GM
      FW(7)=F(7)*RO*G(7)*GM
      BW(7)=B(7)*RO*RO*G(8)*G(8)*GM
      FW(8)=F(8)*RO*G(5)*GM
      BW(8)=B(8)*RO*RO*G(2)*G(2)*GM
      FW(9)=RO*G(9)*GM*F(9)
      BW(9)=B(9)*RO*RO*G(8)*G(2)*GM
      FW(10)=F(10)*RO*G(10)*GM
      BW(10)=B(10)*RO*RO*G(7)*G(2)*GM
      FW(11)=F(11)*RO*G(11)*GM
      BW(11)=B(11)*RO*RO*G(9)*G(2)*GM
      FW(12)=F(12)*RO*G(12)*G(4)
      BW(12)=B(12)*RO*G(13)*G(1)
      FW(13)=F(13)*RO*G(9)*G(2)
      BW(13)=B(13)*RO*G(5)*G(8)
      FW(14)=F(14)*RO*G(9)*G(8)
      BW(14)=B(14)*RO*G(7)*G(2)
      FW(15)=F(15)*RO*G(9)*G(5)
      BW(15)=B(15)*RO*G(11)*G(2)
      FW(16)=F(16)*RO*G(9)*G(9)
      BW(16)=B(16)*RO*G(10)*G(2)
      FW(17)=F(17)*DSQRT(G(14))*G(5)
      IF(TPR(I).GE.6.D2) GO TO 80
      ZZ(I)=ZX/12.
      TO(I)=0.
      IF(T(I).LT.6.D2) GO TO 17
   80 CONTINUE
      IF(TO(I).GE.TAU) GO TO 17
      FW(17)=VO(I)*1.57/TAU*(DSQRT(1.-TO(I)/TAU))/CW(14)
      GO TO 18
   17 FW(17)=0.
   18 BW(17)=0.D0
      IF(IZE.GT.0) FW(17)=0.
      DO 15 M=1,IRE
```

```
      CR(M)=FW(M)-BW(M)
      PRT(M)=(FW(M)*((AF(M)-BF(M))*T(I)+E(M))-BW(M)*((AB(M)-BB(M))*T(I)+
     1D(M)))/(T(I)**2)
   15 CONTINUE
      PRT(IRE)=FW(IRE)*(1.0/(T(I)-555.5)+E(IRE)/(T(I)**2))
      PRT(IRE)=0.
      IF(IZE.GT.0) PRT(IRE)=0.
      IF(KRAS.GT.0) GO TO 3
      IREM1=IRE-1
      DO 71 II=1,ISP
      DO 71 J=1,IREM1
      PK(II,J)= FW(J)*(GNUF(II,J)/G(II)-BF(J)*SM)-BW(J)*(GNUB(II,J)/G(I
     1I)-BB(J)*SM)
      IF(J.GE.5.AND.J.LE.IMU) GO TO 72
      GO TO 71
   72 PK(II,J)=PK(II,J)+(FW(J)-BW(J))/GM
   71 PK(II,J)=PK(II,J)/CW(II)
      DO 73 II=1,ISP
      PK(II,IRE)=0.0
   73 CONTINUE
      IF(IZE.GT.0) GO TO 3
    3 CONTINUE
      IF(KRAS.EQ.0) GO TO 4
      W(1,I)=CW(1)*(-CR(1)+CR(2)+CR(3)+2.0*CR(5)+CR(6)+CR(12))
      W(2,I)=CW(2)*(CR(1)-CR(2)+CR(4)+2.0*CR(8)+CR(9)+CR(10)+CR(11)-CR(1
     13)+CR(14)+CR(15)+CR(16))
      W(3,I)=CW(3)*(CR(3)+CR(4)-CR(6))
      W(4,I)=CW(4)*(CR(1)+CR(2)-CR(3)-2.0*CR(4)+CR(6)-CR(12))
      W(5,I)=CW(5)*(-CR(1)-CR(8)+CR(13)-CR(15)-EN/2.0*CR(17))
      W(6,I)=CW(6)*(-CR(2)-CR(3)-CR(5)+(EN+1.0)*CR(17))
      W(7,I)=CW(7)*(-CR(7)+CR(10)+CR(14))
      W(8,I)=CW(8)*(2.0*CR(7)+CR(9)+CR(13)-CR(14))
      W(9,I)=CW(9)*(-CR(9)+CR(11)-CR(13)-CR(14)-CR(15)-2.0*CR(15))
      W(10,I)=CW(10)*(-CR(10)+CR(16))
      W(11,I)=CW(11)*(-CR(11)+CR(15))
      W(12,I)=CW(12)*(-CR(12)+EN*CR(17))
      W(13,I)=CW(13)*(CR(12))
      W(14,I)=CW(14)*(-CR(17))
      IF(KRAS.GT.0) GO TO 20
    4 CONTINUE
      PT(1)=CW(1)*(-PRT(1)+PRT(2)+PRT(3)+2.0*PRT(5)+PRT(6)+PRT(12))
      PT(2)=CW(2)*(PRT(1)-PRT(2)+PRT(4)+2.0*PRT(8)+PRT(9)+PRT(10)+PRT(11
     1)-PRT(13)+PRT(14)+PRT(15)+PRT(16))
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      PT(3)=CW(3)*(PRT(3)+PRT(4)-PRT(6))
      PT(4)=CW(4)*(PRT(1)+PRT(2)-PRT(3)-2.0*PRT(4)+PRT(6)-PRT(12))
      PT(5)=CW(5)*(-PRT(1)-PRT(8)+PRT(13)-PRT(15)-EN/2.0*PRT(17))
      PT(6)=CW(6)*(-PRT(2)-PRT(3)-PRT(5)+(EN+1.0)*PRT(17))
      PT(7)=CW(7)*(-PRT(7)+PRT(10)+PRT(14))
      PT(8)=CW(8)*(2.0*PRT(7)+PRT(9)+PRT(13)-PRT(14))
      PT(9)=CW(9)*(-PRT(9)+PRT(11)-PRT(13)-PRT(14)-PRT(15)-2.0*PRT(16))
      PT(10)=CW(10)*(-PRT(10)+PRT(16))
      PT(11)=CW(11)*(-PRT(11)+PRT(15))
      PT(12)=CW(12)*(-PRT(12)+EN*PRT(17))
      PT(13)=CW(13)*(PRT(12))
      PT(14)=CW(14)*(-PRT(17))
      DO 21 L=1,ISP
      PA(L,1)=CW(1)*(-PK(L,1)+PK(L,2)+PK(L,3)+2.0*PK(L,5)+PK(L,6)+PK(L,1
     12))
      PA(L,2)=CW(2)*(PK(L,1)-PK(L,2)+PK(L,4)+2.0*PK(L,8)+PK(L,9)+PK(L,10
     1)+PK(L,11)-PK(L,13)+PK(L,14)+PK(L,15)+PK(L,16))
      PA(L,3)=CW(3)*(PK(L,3)+PK(L,4)-PK(L,6))
      PA(L,4)=CW(4)*(PK(L,1)+PK(L,2)-PK(L,3)-2.0*PK(L,4)+PK(L,6)-PK(L,12
     1))
      PA(L,5)=CW(5)*(-PK(L,1)-PK(L,8)+PK(L,13)-PK(L,15)-EN/2.0*PK(L,17))
      PA(L,6)=CW(6)*(-PK(L,2)-PK(L,3)-PK(L,5)+(EN+1.00)*PK(L,17))
      PA(L,7)=CW(7)*(-PK(L,7)+PK(L,10)+PK(L,14))
      PA(L,8)=CW(8)*(2.0*PK(L,7)+PK(L,9)+PK(L,13)-PK(L,14))
      PA(L,9)=CW(9)*(-PK(L,9)+PK(L,11)-PK(L,13)-PK(L,14)-PK(L,15)-2.0*PK
     1(L,16))
      PA(L,10)=CW(10)*(-PK(L,10)+PK(L,16))
      PA(L,11)=CW(11)*(-PK(L,11)+PK(L,15))
      PA(L,12)=CW(12)*(-PK(L,12)+EN*PK(L,17))
      PA(L,13)=CW(13)*(PK(L,12))
      PA(L,14)=CW(14)*(-PK(L,17))
   21 CONTINUE
      IF(KRYS.NE.-10) GO TO 20
   20 CONTINUE
      RETURN
  600 FORMAT(7F10.0)
  601 FORMAT(5E10.4)
  602 FORMAT(9F8.0)
  700 FORMAT(2X,7F14.4)
  701 FORMAT(2X,9E14.4)
  702 FORMAT(2X,9F14.2)
  703 FORMAT('1')
C
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                0.25470497E 05
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 0.90777547E-12 0.29137190E 05
 0.41565016E 01-0.17244334E-02 0.56982316E-05-0.45930044E-08
 0.14233654E-11-0.30288770E 05
 0.38234708E 01-0.11187229E-02 0.12466819E-05-0.21035896E-09
-0.52546551E-13 0.35852787E 04
 0.37189946E 01-0.25167288E-02 0.85837353E-05-0.82998716E-08
 0.27082180E-11-0.10576706E 04
 0.28460849E 01 0.41932116E-02-0.96119332E-05 0.95122662E-08
-0.33093421E-11-0.96725572E 03
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-0.38452940E-15 0.38811792E 04
 0.35976129E 01 0.78149603E-03-0.22386670E-06 0.42490159E-10
-0.33460204E-14-0.11927914E 04
 0.30436897E 01 0.61187110E-03-0.73993551E-08-0.20331907E-10
 0.24593791E-14-0.85491002E 03
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10769.   0.       13712.   3563.    37992.   0.       14090.   0.
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Tullahoma, Tennessee 37388

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13. ABSTRACT

An experimental and theoretical study has been made of the history of the pollutants carbon monoxide (CO), unburned hydrocarbons (HC) and nitrogen oxides (NO_x) in a turbojet afterburner. Experimental traverses at several axial stations were performed in a simulated afterburner in which exhaust from a J-47 combustor can, operated at medium power, was mixed with fuel spray. Experiments were carried out both in a non-bypass and in a bypass configuration (secondary air was mixed with primary exhaust). The non-bypass tests were carried out at high combustor efficiency, and yielded the following: CO = 300 ppm, HC < 10 ppm, NO_x = 100 ppm. In the bypass tests, fuel distribution was non-uniform and combustor efficiency was low. The concentrations obtained were CO = 10000 ppm, HC = 1000 ppm, NO_x = 100 ppm. The theoretical analysis consisted of a computer program for reacting flow with turbulent mixing. The computer program was very slow and therefore of limited usefulness in terms of cost and questionable results, since it could not be checked against experiment. Infrared measurements of NO in the combustion tunnel were attempted. Indications were obtained of NO at the 5.3 micron band, but quantitative measurements were not obtained.

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14. KEY WORDS	LINK A		LINK B		LINK C	
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Turbine engine pollution Exhaust emissions Computer model Pollution						